ESF Exchange Grant REPORT

Dynamical entanglement properties of ultracold quantum gases in the strongly correlated regime

Researcher
Kai Eckert

Receiving Institut
Theoretical Physics Group
Universitat Autònoma de Barcelona

Host
Prof. Dr. Anna Sanpera

Project report – QUDEDIS Exchange Grant

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I. DESCRIPTION OF THE WORK CARRIED OUT AND THE RESULTS OBTAINED

The main aim of the project was to develop, extend, and test tools to simulate the evolution of quantum spin systems and quantum many-body systems in the strongly correlated regime. In a later stage of the project, we want to apply these tool for studies of dynamical properties, and especially entanglement properties, of ultracold quantum gases in optical potentials in the strongly correlated regime.

In what follows we will shortly comment on the numerical methods we have implemented (sec. A). Afterward we will describe the various projects build upon these methods which we have initiated to study spin-systems and especially many-particle bosonic systems in various scenarios (sec. B-D).

A. Development of numerical algorithms to study strongly correlated many-body systems

The major purpose of the stay was to construct efficient numerical algorithms to study the dynamical evolution of strongly correlated many-body systems. To this aim, we implemented algorithms along the line of Matrix Product State (MPS) methods as described by F. Verstraete *et al.* [1], which use entanglement properties of the system to efficiently reduce the size of the Hilbert space. All the programming has been carried out in Matlab, several checks have been done by comparing the numerical results with analytic results for simple cases or with results from exact diagonalization.

Firstly we have constructed an algorithm capable of simulating the non-dissipative dynamics of one-dimensional spin-1/2 systems with open boundary conditions for arbitrary on-site and nearest-neighbor Hamiltonians. This algorithm can be used (i) to study real-time dynamics under time-independent and time-dependent Hamiltonians and (ii) to search for ground states by imaginary time evolution. We have checked the accuracy of the algorithm for both types of applications by comparison with exact results from, e.g., quantum Ising-type Hamiltonians, as well as by comparison to direct diagonalization for small systems.

Secondly we have extended the algorithms to include also periodic boundary conditions, and again we have checked the correctness of the results from real and imaginary time evolution by comparing them with, e.g., analytic results for the XY model.

Thirdly, we have included the possibility to simulate higher spins in the one-dimensional lattice, which especially allows to study systems of bosons by restricting the maximal number of particles per site to a certain fixed value. As a first test we have applied the algorithms to study the transition from the superfluid to the Mott-Insulator phase for the Bose-Hubbard Hamiltonian by calculating the ground state for various values of the parameters of the Hamiltonian. For small system sized we could again use this to compare our findings to results from exact diagonalization.

To go beyond pure one-dimensional systems, we have applied and tested our code for quasi-two-dimensional settings as spin ladders or zig-zag chains. This should allow us to study effects related to frustration, effective magnetic fields, etc. Also it allows, following the lines of [2], to simulate certain types of disorder in a one-dimensional chain in an effective way.

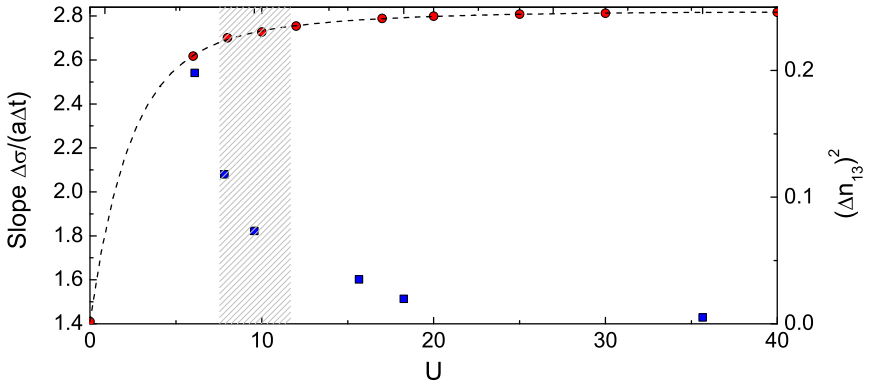

Figure 1: Propagation of an atom injected on top of the multi-particle ground state in a one-dimensional chain of 100 sites as the ratio U/J of on-site interactions U and tunneling J is changed. The red squares show the (constant) slope of the standard deviation and thus the velocity of propagation of the injected atom. Blue squares show the standard deviation of the on-site particle number. The system is in the superfluid (Mott) state for small (large) U/J, the shading indicates the intermediate region.

B. Transport properties in the Bose-Hubbard model

The bose-Hubbard Hamiltonian is a paradigmatic Hamiltonian in condensed matter physics which describes a variety of physical phenomena. For a one dimensional chain it has the form

$$H_{\mathrm{BH}} = -J \sum_{<ij>} \left[\hat{a}_i^\dagger \hat{a}_j + \hat{a}_j^\dagger \hat{a}_i\right] + \frac{U}{2} \sum_i \hat{n}_i(\hat{n}_i - 1) + \mu \sum_i \hat{n}_i, \quad \hat{n}_i = \hat{a}_i^\dagger \hat{a}_i, \tag{1}$$

where $< ij >$ indicates nearest neighbor sites, and $\hat{a}_i^\dagger$ ($\hat{a}_i$) creates (annihilates) a boson at site i. H_{BH} reflects the competition between tunneling of atoms (the term proportional J) and on-site interactions (the term proportional U). An ultracold atomic gas confined in an optical lattice can be brought to form a practically perfect realization of such a Hamiltonian (though usually a shallow confining potential has to be included) [3]. Also several other experimental methods to trap and manipulate cold neutral atoms as, e.g., optical [4, 5] or magnetic microtraps [6, 7], allow – in principle – to realize the Bose-Hubbard Hamiltonian and to control properties as the tunneling between certain chosen sites, or even to construct ”exotic” configurations as ring-shaped or beam splitter-like arrangements. We have started to study especially transport properties in such systems, focusing on the transport of defects (as, e.g., an injected additional particle) on top of the ground state of the Bose-Hubbard Hamiltonian for a certain ratio of on-site interaction and tunneling.

The aims of this project are to study (i) how the type of the underlying ground state – i.e., whether it is superfluid, Mott, or in an intermediate regime – changes transport properties; and (ii) how entanglement can be effectively generated in such a scenario.

With respect to the first point, a simple scenario is to consider the propagation of a single atom injected on top of the ground state of a one dimensional chain. From bosonic enhancement the propagation in the Mott case (i.e., $U/J \to \infty$) is larger by a factor of 2 than in the superfluid case ($U/J \to 0$). As an initial analysis, and also as a further test for our codes, we have studied the transition between both cases for a chain of 100 sites starting from the ground state with

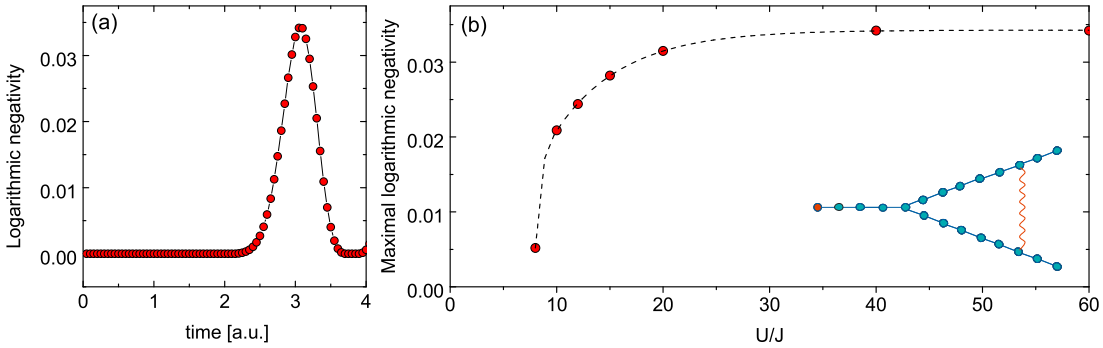

Figure 2: Propagation of an atom injected on top of the multi-particle ground state in a beam-splitter configuration. (a) The logarithmic negativity as a function of time measured in the population number basis for $U/J = 40$ for two nodes, one in each outgoing arm. (b) The maximal logarithmic negativity as U/J is varied between the superfluid and the Mott regime. The inset sketches the beam splitter configuration.

the mean number of particles per site $\langle \hat{n}_i \rangle = 1$ and for different values of the ratio U/J. We assume to inject an additional particle at one site, and calculate how the standard deviation $\sigma = \sqrt{\sum_i (x_i^2 p_i - x_i p_i)}$, $p_i = \langle \hat{n}_i \rangle$, $x_i = ai$, evolves in time. Especially, σ grows linearly in time, and the velocity of propagation is measured by the slope of $\sigma(t)$. As visible in Fig. 1, the slope is nearly constant in the Mott regime, before in the intermediate region it starts to decrease exponentially.

We have also studied different cases as, e.g., ladder-type configurations which allow to include an effective magnetic flux into the system and thus to significantly modify transport properties.

A beam-splitter arrangement (see inset of Fig. 2) allows to produce entanglement between nodes in the two outgoing arms. If an atom is injected into the leftmost node (as before on top of the ground state having a mean number of particles of one per site), it is split at the junction. We use the logarithmic negativity (LN) in the occupation number basis to measure the entanglement generated in this way. Fig. 2 (a) shows how the LN changes in time for $U/J = 40$, i.e., well in the Mott regime, while Fig. 2 (b) give the maximal LN for certain values of U/J. Clearly, the entanglement is largest in the Mott case, and it drops rapidly to zero in the intermediate regime between Mott and superfluid.

After extending these results to include several other situations, a publication is planned in order to summarize the results of this project. Parts of it have been presented in a talk given at the Workshop on Quantum Information at University of Darmstadt (December 2005).

C. Ultracold $F = 2$ spinor gas in an optical lattice in the strongly correlated regime

Recently there has been a strong interest, theoretically as well as experimentally, in ultra-cold atomic spinor gases. As several experimental groups are planning to confine a spinor BEC into an optical lattice, we have studied magnetic properties of the Mott-Insulating phase of $F = 2$ bosons (the $F = 1$ case has been studied in [8]).

The corresponding Hamiltonian has a form similar to the Bose-Hubbard Hamiltonian (1), but

next to the terms representing tunneling and on-site interactions, it contains terms representing the energy associated with spin configurations within one lattice site. In the limit of sufficiently weak tunneling, an effective interaction between neighboring sites can be obtained perturbatively. The ground state of the unperturbed Hamiltonian (zero tunneling) is determined by the scattering lengths for the different channels. Starting from the ground state for one or two particles per site, an effective spin-spin interaction Hamiltonian is obtained, which can be written as a sum of projectors P_S onto states with a certain total spin S:

$$H_I = \sum_{S=0}^{S_{\max}} \lambda_S P_S \,, \tag{2}$$

where all λ_S can be taken non-negative (by adding a number times the unity operator to the Hamiltonian). The energy differences between various channels are again determined by the scattering lengths, and can to some extend be tuned through exploiting Feshbach resonances.

In an optical lattice, tuning the experimental parameters allows to bring the system to a regime of a certain fixed number of atoms per site. States with one or two atoms per lattice site are most interesting, as they do not suffer from three-body losses. For one atom per site, exploiting Feshbach resonances allows extensive control over the parameters of H_I, with the restriction that always $\lambda_1 = \lambda_3$ are largest. For this reason, ground states should belong to the symmetric subspace, and especially we have looked for ground states among ferromagnetic (nematic) states, Néel-type states [9], and valence bond solids with singlets on different pairs (dimers). For certain regions in parameter space, ground states can be easily found in this manifold of states, while in other cases we have applied variational methods. The phase diagram arising in this case (see Fig. 3) can be refined by numerically searching for an MPS minimizing the energy through imaginary time evolution. This allows to identify the region where the ground state is indeed nematic, see the gray region in Fig. 3.

The situation is different for the case of two atoms per site if states with total spin $F = 2$ are assumed as the on-site ground states of the unperturbed Hamiltonian. Then the order of the parameters λ_S in H_I is essentially fixed to be descending, and H_I cannot be tuned as freely through exploiting Feshbach resonances as in the case of one atom per site. For this reason, in this case only ferromagnetically ordered ground states are possible.

A publication summarizing the results of this research project is currently in progress: Ł. Zawitkowski, A. Sanpera, K. Eckert, and M. Lewenstein, *Ultracold atomic $F = 2$ spinor gas in an optical lattice, to be submitted February 2006.*

D. Detection of quantum phase transitions *via* geometric phases

As it has recently been found [10, 11], the geometric phase of the ground state in the spin-1/2 XY model obeys a certain scaling behavior in the vicinity of a quantum phase transition. This behavior, which indeed is a general feature in many-body systems [11], can thus be used to detect quantum phase transitions. A possible advantage with respect to applying Matrix Product States as a numerical tool is that it is not necessary to cross the quantum phase transition to detect it, thus avoiding the region where these tools might not be efficient anymore. We have started to set up algorithms to determine the geometric phase obtained as a loop in parameter spaced is performed around a critical region. We firstly aim at reproducing the result found in [10, 11] for the XX-criticality, before applying it to other criticalities in several models, as to the Ising-criticality in the XY-chain.

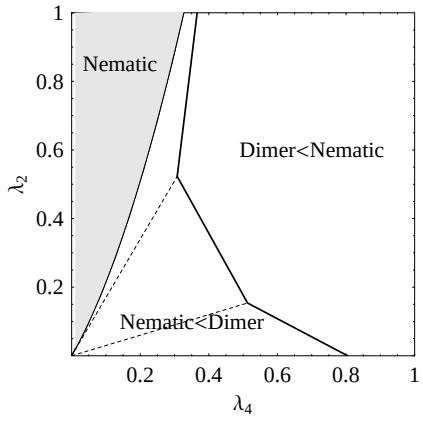

Figure 3: Phase diagram comparing phases with nematic order, Néel order, and valence bond solids with singlets on different pairs (dimers) for the case of a single atom per site. $\lambda_{2,4}$ correspond to the parameters in Hamiltonian 2, furthermore $\lambda_1 = \lambda_3 = 1$, and $\lambda_0 = 0$. Néel-type states turn out to be never optimal. The gray shading indicates the region where the ground state is indeed nematic, as found by numerical imaginary time evolution using MPS in a chain of 50 sites with open boundary conditions.

E. Other results

The support of QUDEDIS has also allowed to finish two other publications which however are not in direct relation with the project:

(i) K. Eckert, J. Mompart, G. Birkl, M. Lewenstein, *Three level atom optics in dipole traps and waveguides*, submitted to Opt. Comm. (2005); also quant-ph/0511195 (2005).

(ii) R. García-Manraver, K. Eckert, R. Corbalán, and J. Mompart, *A deterministic source of polarization entangled photon pairs*, in preparation.

II. FUTURE COLLABORATION

In all the projects listed above, a cooperation between the host and the researcher will continue. With respect to part A the long-term goal is an extension to true two-dimensional systems. With respect to B, we plan to analyze further configurations, e.g., by including spinors or different initial perturbations to the system. Concerning part C we wish to analyze how to detect certain types of ground states in an experiment. Finally, for part D we will study the applicability of our numerical method to the Ising-criticality in the XY model and eventually extend it to other models.

III. FURTHER COMMENTS

KE thanks the Theoretical Physics Group at the Universitat Autònoma de Barcelona for hospitality and J. Calsamigla, J.I. Garcia-Ripoll, M. Lewenstein, J. Mompart, G. Morigi, O. Romero-Isart, A. Sanpera, and Ł. Zawitkowski for many useful discussions.

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